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Diammonium tetrathiocyanatocobaltate(II) tetrahydrate

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(N–C) = 0.008 Å
H-atom completeness 0%
R factor = 0.054
wR factor = 0.177
Data-to-parameter ratio = 20.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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The Co atom of the title compound, $(NH_4)_2[Co(SCN)_4]\cdot 4H_2O$, is located on a special position of site symmetry $\bar{4}$, whereas all atoms of the SCN ligand lie on general positions. As a result, the anions possess crystallographic $\bar{4}$ symmetry. The ammonium cations are located on a twofold rotation axis parallel to *c*. The four water molecules occupy general positions.

Comment

Paramagnetic transition metal complexes are of great importance for the development of new molecule-based magnets and electronic materials. While complexation of Co^{2+} cations with SCN^- ligands leads to tetrahedral high-spin Co^{II} complexes, we became interested in the magnetic properties of the title compound, (I).

$$4\ NH_4SCN + CoCO_3 \xrightarrow[-2NH_3,\ -H_2O]{\text{r. t.}} (NH_4)_2Co(SCN)_4\cdot 4H_2O + CO_2 \qquad \text{(I)}$$

The Co atom is located on a special position of site symmetry $\bar{4}$, whereas the atoms of the SCN ligand lie on general positions. As the result, the anion has crystallographic $\bar{4}$ symmetry. The ammonium cation is located on a twofold rotation axis parallel to *c*. The water molecules occupy general positions.

The packing of the structural components is illustrated in Fig. 2.

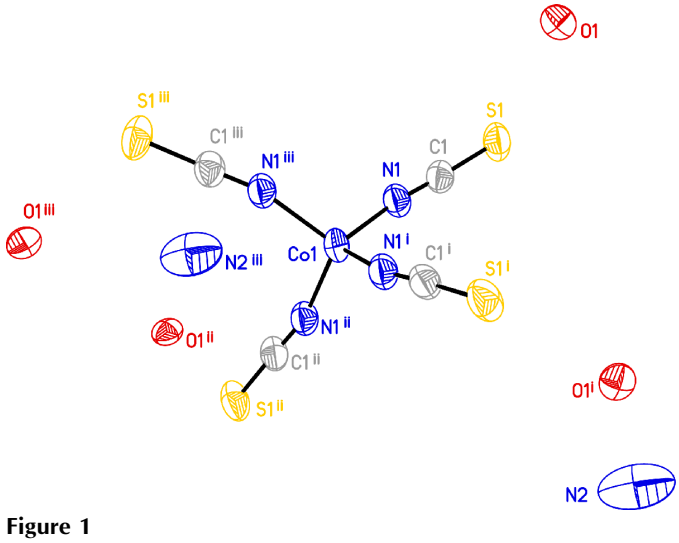

Figure 1
Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. [Symmetry codes: (i) $1-x, 1-y, z$; (ii) $y, 1-x, -z$; (iii) $1-y, x, -z$.]

Experimental

A solution of 9 g NH_4SCN in 100 ml water was dropped into a slurry of 2 g $CoCO_3$ and 50 ml water. After filtering, X-ray quality crystals of the title compound were obtained from the filtrate at ambient temperature.

Crystal data

$(NH_4)_2[Co(SCN)_4]\cdot 4H_2O$
$M_r = 391.33$
Tetragonal, $P\overline{4}2_1c$
$a = 12.2050\ (16)$ Å
$c = 5.3588\ (7)$ Å
$V = 798.26\ (18)$ Å^3
$Z = 2$
$D_x = 1.628$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6680 reflections
$\theta = 3.7$–$27.0°$
$\mu = 1.61$ mm^{-1}
$T = 100$ K
Plate, blue
0.37 × 0.13 × 0.04 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 1990; Blessing, 1995)
$T_{min} = 0.587$, $T_{max} = 0.938$
5438 measured reflections
882 independent reflections
729 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.2°$
$h = -15 \rightarrow 13$
$k = -15 \rightarrow 15$
$l = -6 \rightarrow 6$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.177$
$S = 1.04$
882 reflections
44 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.1367P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.95$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}
Absolute structure: Flack (1983), 351 Friedel pairs
Flack parameter = 0.02 (7)

The H atoms could not be located and were not included in the refinement.

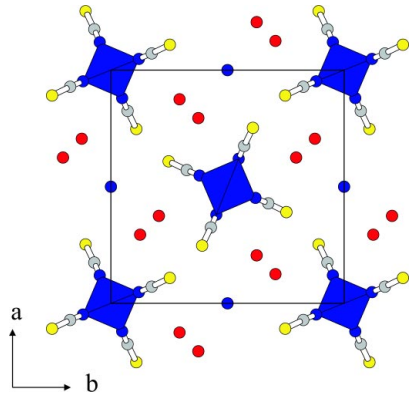

Figure 2
Packing diagram in projection along [001]. Colour code: $[CoN_4]$ tetrahedra blue, N atoms blue, O atoms red, C atoms grey and S atoms yellow.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *PLATON* (Spek, 1990).

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